

Conditional Hamiltonian and Reset Operator in the Quantum Jump Approach¹

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Abstract

For the time development of a single system in the quantum jump approach or for quantum trajectories one requires the conditional (reduced) Hamiltonian between jumps and the reset operator after a jump. Explicit expressions for them are derived for a general N -level system by employing the same assumptions as in the usual derivation of the Bloch equations. We discuss a possible minor problem with positivity for these expressions as well as for the corresponding Bloch equations.
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1. Introduction

In order to better understand photon statistics and photon counting processes for single atoms, in particular the macroscopic dark periods (“electron shelving”) in the Dehmelt V system [1], the quantum jump approach was developed in Göttingen prior to 1991 [2, 3], and consequently analytic aspects were stressed. The independently proposed Monte-Carlo wave function approach [4] is essentially equivalent, but stressed more the computational aspects. The approach by quantum trajectories [5] was also independently proposed and is also essentially equivalent. There are various papers which can be regarded as precursors to the quantum jump approach, in particular Refs. [6, 7]. Some related work [8, 9, 10] on photon statistics will be discussed in Section 5.

Our analytic methods have been applied to interference effects in single atoms [11, 12, 13, 14]. Recently, the quantum jump approach has been extended to study conditional fluorescence spectra, such as the spectrum of an atom in an extended light period [15].

In the derivation of the quantum jump approach one envisages photon measurements in rapid succession at times Δt apart. If a photon is detected at some time it is, for simplicity, assumed to be absorbed. This assumption, however, is not essential [16]. Δt should be much smaller than the level life-times, but it cannot be too small because then one would encounter the quantum Zeno effect [17]; therefore Δt should be larger than the inverse optical frequencies. A reasonable range is $\Delta t \approx 10^{-12}$ s.

Between broadband photon detections the time development of an atom is then described by a reduced, or rather conditional, Hamiltonian H_{cond} , the condition being that no photons are found. It is non-hermitian and allows the calculation of the detection or emission probability. Once a photon is detected, the atomic state has to be reset (a

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“jump”), usually to the ground state, but for general N -level systems the reset states may be quite complicated [3]. Thus the state of a single atom is given by a random path (“quantum trajectory”) determined by the conditional Hamiltonian H_{cond} and the reset states.

In Ref. [3] one of us derived a simple expression for the reset state in the two limiting cases of either widely separated or closely neighbored transition frequencies. The general case seemed to require much smaller Δt ’s, which are difficult to justify physically.

The main purpose of this paper is to re-investigate the reset state using the same methods and approximations as in the derivations of the Bloch equations [18, 8], mainly the Markov approximation. It will be shown that in the general case the (super-)operator which resets the state may depend in a complicated oscillatory way on the choice of Δt . However, this “physical” reset operator can be replaced by a simpler refined or idealized reset operator which gives the same results for all photon counting processes. This idealized reset operator turns out to have the same form as the one obtained in Ref. [3] by using very small Δt ’s. This is explained in detail in Sections 3, while in Section 2 a short derivation of the conditional (or reduced) Hamilton is given. In Section 4 it is shown that the collection of quantum trajectories satisfies the Bloch equations, both for the physical and for the idealized reset operator. In the last section we discuss our results and the positivity of the expressions. It turns out that in some cases the reset operator and the general damping matrix in the conditional Hamiltonian can have a small negative part. A related problem also occurs in Bloch equations where in some examples the solution develops a small negative part for very small times and thus temporarily loses its positivity [19]. But this is probably of no practical relevance.

2. The conditional Hamiltonian H_{cond} for a general N-level system

With an external field $\mathbf{E}_e(t)$, the Hamiltonian for complete system, atom plus quantized electromagnetic field $\mathbf{E} = \mathbf{E}^{(+)} + \mathbf{E}^{(-)}$, is given in the Schrödinger picture, in the limit of long wave-lengths and in the rotating-wave approximation, by [20]

$$\begin{aligned} H &= \sum \hbar \omega_i |i\rangle \langle i| + H_F^0 + [e \mathbf{D}^{(-)} \cdot \mathbf{E}_e^{(+)}(t) + \text{h.c.}] + [e \mathbf{D}^{(-)} \cdot \mathbf{E}^{(+)} + \text{h.c.}] \\ &\equiv H_A^0 + H_F^0 + H_{AL}(t) + H_{AF} \end{aligned} \quad (1)$$

where

$$\begin{aligned} \mathbf{D}^{(-)} &= \sum_{i>j} \mathbf{D}_{ij} |i\rangle \langle j| \\ \mathbf{D}_{ij} &= \langle i | \mathbf{X} | j \rangle \\ \mathbf{E}^{(+)} &= \sum_{\mathbf{k}\lambda} ie \left\{ \frac{\hbar \omega_{\mathbf{k}}}{2\varepsilon_0 V} \right\}^{1/2} \varepsilon_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda}. \end{aligned} \quad (2)$$

and a frequency cutoff is included. V is the quantization volume, later taken in infinity, and $i > j$ means $\omega_i > \omega_j$.

Now one imagines that photon measurements are performed at times $t_1 = \Delta t, t_2 = 2\Delta t, \dots$ on an ensemble of systems which, at time $t = 0$, is supposed to be in the initial state $|0_{ph}\rangle|\psi\rangle$. By the von Neumann - Lüders projection postulate [21] the *subensemble*

for which no photons are detected until time t_n is described, with $P_0 \equiv |0_{ph}\rangle \mathbf{1}_A \langle 0_{ph}|$, by

$$P_0 U(t_n, t_n - \Delta t) P_0 \cdots P_0 U(t_1, 0) |0_{ph}\rangle |\psi\rangle \equiv |0_{ph}\rangle U_{\text{cond}}(t_n, 0) |\psi\rangle . \quad (3)$$

The norm squared of this is the probability of finding no photons for the measurements between 0 and t_n . U_{cond} gives the time development of an atom under the condition that no photon is observed until time t , and it will now be determined explicitly by simple second order perturbation theory. Going over to the interaction picture with respect to $H_A^0 + H_F^0$ one has

$$H_I(t) = H_{AL}^I(t) + H_{AF}^I(t) \quad (4)$$

which is obtained by replacing $|i\rangle\langle j|$ and $a_{\mathbf{k}\lambda}$ in the original interaction Hamiltonian by $|i\rangle\langle j|e^{i\omega_{ij}t}$ and $a_{\mathbf{k}\lambda}e^{-i\omega_{\mathbf{k}\lambda}t}$, respectively, with

$$\omega_{ij} \equiv \omega_i - \omega_j .$$

We now calculate, for $t_i \leq t' < t_{i+1}$,

$$\langle 0_{ph} | \frac{d}{dt'} U_I(t', t_i) | 0_{ph} \rangle . \quad (5)$$

In the first-order contribution only $H_{AL}^I(t)$ remains since

$$\langle 0_{ph} | H_{AF}^I(t) | 0_{ph} \rangle = 0 . \quad (6)$$

The second order is, by Eq. (6),

$$-\hbar^{-2} \int_{t_i}^{t'} dt'' \left\{ \langle 0_{ph} | H_{AF}^I(t') H_{AF}^I(t'') | 0_{ph} \rangle + H_{AL}^I(t') H_{AL}^I(t'') \right\} . \quad (7)$$

Now, if the external field $\mathbf{E}_e(t)$ is smooth in time, e.g. given by laser, and *not* wildly fluctuating like a thermal or chaotic field, then the second part in Eq. (7) contributes a term of higher order in Δt and can therefore be omitted. For a chaotic external field, however, this part may give rise to a contribution of the same order and then has to be retained. In this case one can no longer work with state vectors (“wave functions”) but has to use (conditional) density matrices. A particular example of this is treated in Ref. [12].

Thus, supposing a smooth external field, the second-order contribution becomes

$$\begin{aligned} & -\hbar^{-2} \int_{t_i}^{t'} dt'' \sum_{\substack{ij\ell m \\ i>j, \ell>m}} |i\rangle\langle j|m\rangle\langle\ell| \sum_{\mathbf{k}\lambda} \frac{e^2 \hbar \omega_k}{2\epsilon_0 V} (\mathbf{D}_{ij} \cdot \boldsymbol{\varepsilon}_{\mathbf{k}\lambda}) (\boldsymbol{\varepsilon}_{\mathbf{k}\lambda} \cdot \mathbf{D}_{m\ell}) e^{-i(\omega_{\mathbf{k}} - \omega_{ij})t' + i(\omega_{\mathbf{k}} - \omega_{\ell m})t''} \\ &= -\hbar^{-2} \sum_{\substack{ij\ell \\ i,\ell>j}} e^{i(\omega_{ij} - \omega_{\ell j})t'} |i\rangle\langle\ell| \int_0^{t'-t_i} d\tau \sum_{\mathbf{k}\lambda} \frac{e^2 \hbar \omega_k}{2\epsilon_0 V} (\mathbf{D}_{ij} \cdot \boldsymbol{\varepsilon}_{\mathbf{k}\lambda}) (\boldsymbol{\varepsilon}_{\mathbf{k}\lambda} \cdot \mathbf{D}_{j\ell}) e^{-i(\omega_{\mathbf{k}} - \omega_{\ell j})\tau} . \end{aligned} \quad (8)$$

One can now use properties of the correlation function

$$\kappa_{jilm}(\tau) \equiv \sum_{\mathbf{k}\lambda} \frac{e^2 \omega_{\mathbf{k}}}{2\epsilon_0 \hbar V} (\mathbf{D}_{ji} \cdot \boldsymbol{\varepsilon}_{\mathbf{k}\lambda}) (\boldsymbol{\varepsilon}_{\mathbf{k}\lambda} \cdot \mathbf{D}_{lm}) e^{-i(\omega_{\mathbf{k}} - \omega_{\ell m})\tau} . \quad (9)$$

With $V^{-1} = \Delta^3 k / (2\pi)^3$ one can perform the limit $V \rightarrow \infty$, and the sum over \mathbf{k} becomes an integral over ω , with a suitable frequency cutoff, and an integral over the unit sphere. The correlation function has an effective width of the order of $\omega_{\ell m}^{-1}$ around $\tau = 0$, and for $t' - t_i \gg \omega_{\ell m}^{-1}$ one can therefore extend the τ integration in Eq. (8) to infinity [22]. This is equivalent to the approximation

$$\int_0^{t'-t_i} d\tau e^{i(\omega_{\ell m} - \omega_{\mathbf{k}})\tau} \cong \pi\delta(\omega_{\mathbf{k}} - \omega_{\ell m}) + i\mathcal{P}\frac{1}{\omega_{\mathbf{k}} - \omega_{\ell m}} \quad (10)$$

and corresponds to the usual Markov approximation in the derivation of the Bloch equations [18, 8]. For the second-order contribution one then obtains

$$-\sum_{\substack{ij\ell \\ i,\ell>j}} |i\rangle\langle\ell| e^{i\omega_{i\ell}t'} \int d^3k \frac{e^2\omega_{\mathbf{k}}}{(2\pi)^3\hbar 2\epsilon_0} \mathbf{D}_{ij} \cdot \sum_{\lambda=1}^2 \varepsilon_{\mathbf{k}\lambda} \varepsilon_{\mathbf{k}\lambda} \cdot \mathbf{D}_{j\ell} (\pi\delta(\omega_{\mathbf{k}} - \omega_{\ell m}) + i\mathcal{P}\frac{1}{\omega_{\mathbf{k}} - \omega_{\ell m}}). \quad (11)$$

The principal-value term is analogous to a level shift and is often omitted [8, 23]. The last integral equals $\Gamma_{ijj\ell}$ where

$$\Gamma_{ijk\ell} \equiv \frac{e^2}{6\pi\epsilon_0\hbar c^3} \mathbf{D}_{ij} \cdot \mathbf{D}_{k\ell} |\omega_{k\ell}|^3 + \text{principal value term} \quad (12)$$

Hence, integrating over t' from t_i to t_{i+1} and using $1 + \delta \approx e^\delta$ for small δ , we obtain

$$\langle 0_{ph} | U_I(t_{i+1}, t_i) | 0_{ph} \rangle = \exp \left\{ -\frac{i}{\hbar} \int_{t_i}^{t_{i+1}} dt' \left\{ H_{AL}(t') - i\hbar \sum_{\substack{ij\ell \\ i,\ell>j}} \Gamma_{ijj\ell} e^{i\omega_{i\ell}t'} |i\rangle\langle\ell| \right\} \right\}. \quad (13)$$

For small Δt this can be replaced by a time-ordered exponential and thus, with $t = t_n$,

$$\prod_1^n \langle 0_{ph} | (U_I(t_i, t_{i-1})) | 0_{ph} \rangle \cong \mathcal{T} \exp \left\{ -\frac{i}{\hbar} \int_0^t dt' \left\{ H_{AL}(t') - i\hbar \sum_{\substack{ij\ell \\ i,\ell>j}} \Gamma_{ijj\ell} e^{i\omega_{i\ell}t'} |i\rangle\langle\ell| \right\} \right\} \quad (14)$$

where the product sign on the l.h.s. includes an ordering in an obvious way.

Since

$$\langle 0_{ph} | U(t_i, t_{i-1}) | 0_{ph} \rangle = e^{-iH_A^0 t_i/\hbar} \langle 0_{ph} | U_I(t_i, t_{i-1}) | 0_{ph} \rangle e^{iH_A^0 t_{i-1}/\hbar} \quad (15)$$

and since, for $t = t_n = n\Delta t$,

$$U_{\text{cond}}(t, 0) = \prod_1^n \langle 0_{ph} | U(t_i, t_{i-1}) | 0_{ph} \rangle,$$

we obtain, on a coarse-grained time scale, from Eqs. (14) and (15)

$$U_{\text{cond}}(t, 0) = \mathcal{T} \exp \left\{ -\frac{i}{\hbar} \int_0^t dt' \left\{ H_A^0 + H_{AL}(t') - i\hbar \sum_{\substack{ij\ell \\ i,\ell>j}} \Gamma_{ijj\ell} |i\rangle\langle\ell| \right\} \right\} \quad (16)$$

which is the transformation of Eq. (14) back to the Schrödinger picture.

Thus, with the atomic operator Γ defined as

$$\Gamma \equiv \sum_{\substack{i,j \\ i,\ell > j}} \Gamma_{ijj\ell} |i\rangle\langle\ell| \quad (17)$$

the conditional Hamiltonian for an N -level atom with no photon emission until time t is, on the coarse-grained time scale, given by

$$H_{\text{cond}}(t) = H_A^0 + H_{AL}(t) - i\hbar\Gamma. \quad (18)$$

For initial atomic state $|\psi\rangle$ the probability to find no photon until time t is thus given by

$$\|U_{\text{cond}}(t, 0)|\psi\rangle\|^2, \quad (19)$$

and the probability to find the first photon in $(t, t + \Delta t)$ is the difference of this expression for t and $t + \Delta t$. Thus, on the coarse grained time scale the probability density $w(t)$ for the first photon is the negative derivative of Eq. (18),

$$\begin{aligned} w(\tau) &= -\frac{d}{dt} \|U_{\text{cond}}(t, 0)|\psi\rangle\|^2 \\ &= \langle\psi|\Gamma + \Gamma^*|\psi\rangle. \end{aligned} \quad (20)$$

When one lets Δt become smaller and smaller the above derivation shows very nicely how and where the quantum Zeno effect [17] turns up in a very natural way. If Δt is chosen much smaller than the inverse optical frequencies, the last exponential in Eq. (8) can be replaced by 1, and the integral becomes proportional to $t' - t_i$. Eq. (13) is then replaced by

$$\langle 0_{ph}|U_I(t_{i+1}, t_i)|0_{ph}\rangle = \exp \left\{ -\frac{i}{\hbar} \left\{ H_{AL}(t_i)\Delta t - i\hbar \text{ const } \sum_{\substack{i,j,\ell \\ i,\ell > j}} \Gamma_{ijj\ell} e^{i\omega_{i\ell} t_i} |i\rangle\langle\ell| (\Delta t)^2 \right\} \right\}. \quad (21)$$

The product of these operators then becomes, for $\Delta t \rightarrow 0$,

$$\mathcal{T} \exp \left\{ -\frac{i}{\hbar} \int_0^t dt' \{H_{AL}(t')\} \right\}. \quad (22)$$

This is a purely atomic operator, and hence the time development of the field becomes frozen, i. e. for $\Delta t \rightarrow 0$ one always remains in the vacuum. For this reason one cannot choose Δt arbitrarily small in the quantum jump approach.

3. The reset operator

In this section we determine the state (or density matrix) of an atom after a broadband detection of a photon, under the condition that shortly before no photon was found. We therefore consider an ensemble where no photon are present at time t_n . The ensemble is thus described by $\rho(t_n) = |0_{ph}\rangle\rho_A(t_n)\langle 0_{ph}|$ where ρ_A is the density matrix of the atoms.

The state of the subensemble for which photons are detected by a non-absorptive measurement at time $t_{n+1} = t_n + \Delta t$ is given, in view of the von Neumann-Lüders projection postulate [21], by

$$P_1\rho(t_{n+1})P_1/\text{tr}(\cdot) \quad (23)$$

where

$$P_1 \equiv \mathbf{1} - |0_{ph}\rangle\langle 0_{ph}|. \quad (24)$$

Note that Eq. (23) still contains the photons.

After a photon measurement by absorption no photons are present any longer and it was argued in Ref. [3] that the resulting reset state is obtained from Eq. (23) by a partial trace over the photons, i.e. by

$$|0_{ph}\rangle (\text{tr}_{ph} P_1 \rho(t_{n+1}) P_1) \langle 0_{ph}|/\text{tr}(\cdot). \quad (25)$$

The physical reason for this is that for the atomic description alone it should make no difference in infinite space whether or not the photons are absorbed, as long as they are sufficiently far away from the atom and no longer interacting with it [24]. Eq. (25) can be calculated by perturbation theory for $U_I(t_{n+1}, t_n)$, as in Section 2. Now, the first-order contribution suffices and one obtains in a straightforward way for the reset state

$$\begin{aligned} \hat{\mathcal{R}}(\Delta t)\rho_A(t_n) &\equiv \text{tr}_{ph} P_1 U(t_{n+1}, t_n) |0_{ph}\rangle \rho_A(t_n) \langle 0_{ph}| U(t_{n+1}, t_n)^* P_1 \\ &= e^{-iH_A^0 \Delta t / \hbar} \sum_{\substack{ij\ell m \\ i>j, \ell>m}} |j\rangle \langle i| \rho_A(t_n) |\ell\rangle \langle m| e^{iH_A^0 \Delta t / \hbar} \\ &\times \int_0^{\Delta t} dt' \int_0^{\Delta t} dt'' e^{i\omega_{\mathbf{k}}(t'-t'') - i\omega_{ij}t' + i\omega_{\ell m}t''} \sum_{\mathbf{k}\lambda} \frac{e^2 \omega_{\mathbf{k}}}{2\varepsilon_0 \hbar V} (\mathbf{D}_{ji} \cdot \varepsilon_{\mathbf{k}\lambda}) (\varepsilon_{\mathbf{k}\lambda} \cdot \mathbf{D}_{\ell m}). \end{aligned} \quad (26)$$

Note that the atomic trace $\text{tr}_A \hat{\mathcal{R}}(\Delta t)\rho_A(t_n)$ gives the probability for a photon to be found at time t_{n+1} under the condition that no photons were found at time t_n .

The external field drops out in the first-order contribution since its action during the short time Δt is of second order only. To apply the Markov property, we decompose the rectangular integration domain over t' and t'' in Eq. (26) into two triangles, leading to [25]

$$\int_0^{\Delta t} dt' e^{-i(\omega_{ij} - \omega_{\ell m})t'} \int_0^{t'} dt'' e^{i(\omega_{\mathbf{k}} - \omega_{\ell m})(t' - t'')} + \int_0^{\Delta t} dt'' e^{-i(\omega_{ij} - \omega_{\ell m})t''} \int_0^{t''} dt' e^{-i(\omega_{\mathbf{k}} - \omega_{ij})(t'' - t')} . \quad (27)$$

As in Eqs. (8) and (10) the inner integrals can be replaced by $\pi\delta(\omega_{\mathbf{k}} - \omega_{\ell m})$ and $\pi\delta(\omega_{\mathbf{k}} - \omega_{ij})$, respectively, plus principal values. In the limit $V \rightarrow \infty$ the sum over \mathbf{k} becomes an integral over $d^3 k$ as in Eq. (11). With Γ_{ijkl} given by Eq. (12) we thus obtain

$$\hat{\mathcal{R}}(\Delta t)\rho_A(t_n) = e^{-iH_A^0 \Delta t / \hbar} \sum_{\substack{ij\ell m \\ i>j, \ell>m}} \{\Gamma_{jilem} + \Gamma_{\ell mji}\} |j\rangle \langle i| \rho_A(t_n) |\ell\rangle \langle m| e^{iH_A^0 \Delta t / \hbar} \int_0^{\Delta t} dt' e^{-i(\omega_{ij} - \omega_{\ell m})t'} \quad (28)$$

Up to normalization this is the state of an atom after a photon detection at time $t_n + \Delta t$, under the condition that no photons were found at time t_n . Its trace gives the probability for this event.

Even after normalization the state will in general depend in an oscillatory way on Δt , except in two limiting cases which were discussed in Ref. [3]. If two optical transition frequencies ω_{ij} and $\omega_{\ell m}$ are far apart, then $|\omega_{ij} - \omega_{\ell m}| \Delta t \gg 1$ and the integral in Eq. (28) vanishes. The other case is when two optical transition frequencies are very close so that $|\omega_{ij} - \omega_{\ell m}| \Delta t \ll 1$. Then the integral in Eq. (28) is essentially 1, and in this case one may obtain interesting coherence effects which were discussed for the Λ system in Ref. [13].

There is a close connection between the reset operator, the conditional Hamiltonian, and the Bloch equations. By Eq. (24) one can write Eq. (25) for the reset state as

$$\text{tr}_{ph} P_1 \rho(t_{n+1}) = \text{tr}_{ph} U(t_{n+1}, t_n) \rho(t_n) U(t_{n+1}, t_n)^* - \langle 0_{ph} | U(t_{n+1}, t_n) \rho(t_n) U(t_{n+1}, t_n)^* | 0_{ph} \rangle \quad (29)$$

with $\rho(t_n) = |0_{ph}\rangle \rho_A(t_n) \langle 0_{ph}|$. The first term on the right hand side is the definition of the atomic density matrix in the Bloch equations, while the second is given by the conditional time development operator. Hence one can obtain the reset operator also from a knowledge of the Bloch equations and H_{cond} .

For the general case the reset operator in Eq. (28) is cumbersome to work with, and it will now be shown that one can replace it by a refined – and simpler – expression which gives equivalent results for all photon counting questions.

We define the atomic superoperator \hat{J} by

$$\hat{J} \rho_A \equiv \sum_{\substack{ij\ell m \\ i>j, \ell>m}} \{ \Gamma_{j\ell m} + \Gamma_{\ell m j i} \} |j\rangle \langle i| \rho_A |\ell\rangle \langle m| . \quad (30)$$

Formally one has

$$\hat{J} = \lim_{\Delta t \rightarrow 0} \hat{\mathcal{R}}(\Delta t) / \Delta t \quad (31)$$

but of course this limit is not really physically allowed. However, the photon counting probabilities obtained from \hat{J} for physically allowed Δt 's turn out to be in agreement with those obtained from $\hat{\mathcal{R}}(\Delta t)$.

As in Ref. [3] we define the atomic superoperator $\hat{S}(t, t_0)$ by

$$\hat{S}(t, t_0) \rho_A \equiv U_{\text{cond}}(t, t_0) \rho_A U_{\text{cond}}(t, t_0)^* . \quad (32)$$

Based on \hat{J} as reset operator the probability density $w(\tau_1, \dots, \tau_k; [0, t])$ for finding a photon exactly at the times τ_1, \dots, τ_k in $[0, t]$ is given by [3]

$$w(\tau_1, \dots, \tau_k; [0, t]) = \text{tr}_A (\hat{S}(t, \tau_k) \hat{J} \hat{S}(\tau_k, \tau_{k-1}) \hat{J} \dots \hat{J} \hat{S}(\tau_1, 0_1) \rho_A(0)) \quad (33)$$

To see how this compares with the photon counting probabilities obtained from $\hat{\mathcal{R}}(\Delta t)$ we first express the latter by means of \hat{J} as follows. Let $\hat{T}_0(t, t_0)$ be the superoperator for the *free* time evolution of atomic density matrices,

$$\hat{T}_0(t, t_0) \rho_A \equiv e^{-iH_A^0(t-t_0)/\hbar} \rho_A e^{iH_A^0(t-t_0)/\hbar} \quad (34)$$

and let $\hat{T}(t, t_0)$ be the time evolution including driving and damping, i.e. given by the solution of the Bloch equations. With \hat{T}_0 Eq. (28) can obviously be written as

$$\hat{\mathcal{R}}(\Delta t) = \int_0^{\Delta t} dt' \hat{T}_0(\Delta t - t', 0) \hat{J} \hat{T}_0(t', 0) . \quad (35)$$

We now use this expression for $\hat{\mathcal{R}}(\Delta t)$ to calculate the probability of finding a photon in the small time interval $[t_i, t_{i+1}]$ and none between 0 and t_i and none between t_{i+1} and t . With a simple change of integration range in Eq. (35) the desired probability is given by

$$\text{tr}_A \hat{S}(t, t_{i+1}) \hat{\mathcal{R}}(\Delta t) \hat{S}(t_i, 0) \rho_A(0) = \int_{t_i}^{t_{i+1}} d\tau_1 \text{tr}_A \hat{S}(t, t_{i+1}) \hat{T}_0(t_{i+1}, \tau_1) \hat{J} \hat{T}_0(\tau_1, t_i) \hat{S}(t_i, 0) \rho_A(0). \quad (36)$$

Now, since $\Delta t = t_{n+1} - t_n$ is small compared to the inverse damping and driving, one may – during Δt – replace \hat{T}_0 by \hat{T} or by \hat{S} . Here we replace it by \hat{S} and obtain for Eq. (36)

$$\int_{t_i}^{t_{i+1}} d\tau_1 \text{tr}_A (\hat{S}(t, \tau_1) \hat{J} \hat{S}(\tau_1, 0) \rho_A(0)). \quad (37)$$

The integrand is just the probability density $w(\tau_1; [0, t])$ of Eq. (33) associated with \hat{J} for $k = 1$. It is clear that this argument immediately carries over to more than a single photon detection. The essential point is seen to be the fact that during a single time interval Δt the damping has negligible effect.

We thus have shown that for all photon countings we can use the refined – or idealized – reset operator \hat{J} and the densities of Eq. (33).

4. Connection with Bloch Equations

In Ref. [3] it had been shown that an ensemble of atoms whose individual time development proceeded according to H_{cond} and the reset operator \hat{J} after photon detections (“jumps”) also obeys the Bloch equations. If instead one uses the reset operator $\hat{\mathcal{R}}(\Delta t)$ from Eq. (28), to what extent do the Bloch equations still hold?

The subensemble of atoms with no photons until t is described by $\hat{S}(t, 0) \rho_A(0)$ and the subensemble with last photon detection before t at time t_i by

$$\hat{S}(t, t_i) \hat{\mathcal{R}}(\Delta t) \rho_A(t_{i-1})$$

where $t = n\Delta t$ and $t_i = i\Delta t$. Thus the complete ensemble of atoms is described at time t by

$$\rho_A(t) = \hat{S}(t, 0) \rho_A(0) + \sum_{i=1}^{n-1} \hat{S}(t, t_i) \hat{\mathcal{R}}(\Delta t) \rho_A(t_{i-1}).$$

With Eq. (35) and a change of integration variable one obtains

$$\rho_A(t) = \hat{S}(t, 0) \rho_A(0) + \sum_{i=1}^{n-1} \int_{t_i}^{t_{n+1}} d\tau \hat{S}(t, t_i) \hat{T}_0(t_i, \tau) \hat{J} \hat{T}_0(\tau, t_{i-1}) \rho_A(t_{i-1}). \quad (38)$$

As noticed before, during a single time interval Δt the driving and damping has negligible effect, and therefore one can replace in Eq. (38), for this short time interval, $\hat{T}_0(t_i, \tau)$ by $\hat{S}(t_i, \tau)$ and $\hat{T}_0(\tau, t_{i-1})$ by $\hat{T}(\tau, t_{i-1})$, where the latter is the time development operator of the Bloch equations including driving and damping. Since $\hat{T}(\tau, t_{i-1}) \rho_A(t_{i-1}) = \rho_A(\tau)$, one obtains with this approximation

$$\rho_A(t) = \hat{S}(t, 0) \rho_A(0) + \sum_{i=1}^{n-1} \int_{t_i}^{t_{i+1}} d\tau \hat{S}(t, \tau) \hat{J} \rho_A(\tau)$$

and thus

$$\rho_A(t) = \hat{S}(t, 0)\rho_A(0) + \int_0^t d\tau \hat{S}(t, \tau)\hat{J}\rho_A(\tau) \quad (39)$$

which is just the equation one would have obtained with \hat{J} as reset operator. Introducing a coarse-grained time scale one can now differentiate with respect to t and obtains

$$\dot{\rho}_A = -\frac{i}{\hbar} \{H_{\text{cond}}\rho_A(t) - \rho_A(t)H_{\text{cond}}^*\} + \hat{J}\rho_A(t)$$

which agrees with the usual Bloch equations [8].

5. Discussion

The idea of the quantum jump approach is to describe the radiating atom between photon detections by a conditional (or reduced) time evolution operator giving the time development under the condition that no photon has been detected. After a photon detection one has to reset the atom to the reset state ("jump"), with ensuing reduced time development, and so on. For a driven system with many emissions one then obtains a stochastic path ("quantum trajectory"). An ensemble of such paths for an ensemble of driven atoms satisfies the Bloch equations. In fact both quantum trajectories and Bloch equations are possible and equivalent ways to describe the time evolution of an ensemble of fluorescing atoms, but the former is also easy to apply to the emission behavior of a single atom.

As outlined above the photon measurements are taken at rapidly repeated discrete times. On a coarse-grained time-scale the paths can be regarded as continuous, and the quantum jump approach can be considered as a simple model for continuous measurements. The photon operators \hat{S} and \hat{J} for the photon counting distributions of Sections 3 in general not only satisfy all the requirements of the axiomatic continuous-measurement theory of Ref. [10], but are explicitly given, in contrast to the axiomatic theory where they have to be more or less guessed. In some cases positivity problems for \hat{S} and \hat{J} can arise, as discussed further below.

In Ref. [8] $\|P_0 U(t, 0)|0_{ph}\rangle|\psi\rangle\|^2$, the no-photon probability *at* time t was calculated, i.e. $= \|\langle 0_{ph}|U(t, 0)|0_{ph}\rangle|\psi\rangle\|^2$, which is, in principle, different from the probability of finding no photon *until* time t , since in the latter case one has to measure in between. Interestingly, though, Ref. [8] finds for the no-photon probability *at* time t the same expressions we do for the probability *until* time t , except for their use of $\mathbf{p} \cdot \mathbf{A}$ coupling [24]. This seems to indicate that the reductions used in Eq. (3) are closely related to the Markov assumption and can be replaced by it. Ref. [9] derives photon counting statistics by an approach which can be regarded as an alternative to that of Ref. [2, 3] and which uses the projector formalism together with the Markov property, considering only finite macroscopic time intervals. Interruptions by numerous hypothetical measurements are not needed, and neither is the notion of continuous measurements.

The approximations used in the previous sections are the same as those employed in the usual derivations of the Bloch equations [18, 8], in particular the use of the Markov property, i.e. the fact that the correlation function $\kappa(\tau)$ is very narrowly peaked and drops off rapidly. This is a standard assumption in the derivation of Bloch equations [18, 8, 23].

The integration of the approximated time derivatives over t' from t_i to t_{i+1} in Eq. (13) introduces an error for small $t' - t_i$, just as in the derivation Bloch equations [26], and a similar error occurs in the reset operator. The omission of the principal values in Eqs. (18) and (30) is not necessary. If one retains them, as for example in Ref. [18], only the form of the $\Gamma_{ij\ell m}$'s will be changed. The conditional Hamiltonian will then acquire an additional term through Γ , and Eq. (18) should be written in terms of the hermitian (real) part Γ_r and antihermitian (imaginary) part Γ_i as

$$H_{\text{cond}} = H_A(t) + \Gamma_i - i\Gamma_r . \quad (40)$$

The imaginary part of Γ then contributes to the level shifts, but the effect of its possible non-diagonal parts deserves closer examination, both for the quantum jump approach and for the Bloch equations.

As seen from Eqs. (25) and (26), the reset superoperator must preserve positivity, i.e. must map positive operators onto positive operators. The question is whether, after the approximations used in its derivation, this property still holds. Without explicit calculation of the principal value terms in $\Gamma_{ij\ell m}$ little can be said. However, if one drops the principal value terms, as in the Bloch equations of Ref. [8], then positivity may be lost. In fact, for parallel transition dipole moments the reset matrix of the Λ system [27] calculated from Eq. (30) then has a tiny negative part for small level separation.

Similarly, if the transition to a continuous coarse-grained time scale for the conditional no-photon time development is possible, then Eq. (20) for the probability density of the first photon shows that the hermitian (real) part Γ_r of Γ should be a positive operator. Without explicit calculation of the principle value part little can be said, but if these are omitted then positivity of Γ_r is lost in some cases when Γ has non-diagonal elements, e.g. for a V system with parallel transition dipole moments.

These deviations from positivity are probably small in practical applications. But it would be preferable to work with expressions which do respect positivity. One way to arrive at such expressions is to note that in Eq. (30) for \hat{J} one has, with omission of the principal value terms in $\Gamma_{ij\ell m}$,

$$\Gamma_{jilm} + \Gamma_{\ell m j i} \sim \mathbf{D}_{ji} \cdot \mathbf{D}_{\ell m} \frac{1}{2} (\omega_{ij}^3 + \omega_{\ell m}^3) . \quad (41)$$

Now, if one replaces the arithmetic mean $\frac{1}{2} (\omega_{ij}^3 + \omega_{\ell m}^3)$ by the geometric mean $\sqrt{\omega_{ij}^3 \omega_{\ell m}^3}$ then it is easily seen that positivity of the resulting reset operator is automatic.

Since $\text{tr} \hat{J} \rho_A$ gives the probability density for the first photon, one has, by Eq. (20),

$$\text{tr}(\hat{J} \rho_A) = \text{tr}(\Gamma + \Gamma^*) \rho_A \quad (42)$$

if the coarse-grained time scale can be used. Once one has obtained a positivity preserving \hat{J} one can use Eq. (42) to find a positive Γ_r . A systematic procedure to obtain a positivity preserving expression for the reset operator would be desirable.

In view of the close connection of the quantum jump approach with the Bloch equations it stands to reason that the possible non-positivity of the reset matrix and the damping operator could have its counterpart in the Bloch equations. Indeed, at least if one omits the principal value parts, as in Ref. [8], this can happen for very short times. E.g., for the Λ system with no external driving field and with parallel transition dipole moments one can start initially in the upper state which then, under the time evolution under

the Bloch equations, develops a small negative part for times of the order of the inverse optical frequencies or less, but regains positivity for times larger than that. We have also found that a similar phenomenon happens for a V system with parallel transition dipole moments. Positivity in the Bloch equations is ensured if one makes the replacement of the arithmetic mean in Eq. (41) by the geometric mean. Although this may mean in some cases a substantial change of some coefficients in the Bloch equations, the effect on the behavior of the solutions is expected to be minimal. A similar non-positivity has been found in Ref. [19].

This seems to be similar to the effect of the rotating-wave approximation. Keeping or not keeping the rapidly rotating terms makes some coefficients considerably different, but has little effect on the solutions. For the same reason rapidly oscillatory terms arising through contributions from $\Gamma_{ijj\ell}$ for large $\omega_{j\ell}$ can be omitted. We have kept them here only to exhibit the symmetry of the formulas.

The derivations in this paper were based on the $\mathbf{E} \cdot \mathbf{D}$ coupling. If one uses the $\mathbf{p} \cdot \mathbf{A}$ coupling the results are the same except that the expression for the $\Gamma_{ij\ell m}$ are slightly different. If one again replaces the arithmetic by the geometric mean the results become the same.

In conclusion one may say that the degree of reliability of our results for the conditional (reduced) Hamiltonian and the reset operator is the same as that of the corresponding Bloch equations. Because the times involved are very short – in fact of the order of the correlation time used in the Markov approximation – and the non-positivity very small, there are probably no practical consequences.

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